N-Methylcarbamic acid, ethyl ester 105-40-8 | DTXSID2031746

Model Performance

Mode	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 2.01

Global applicability domain: Inside

Local applicability domain index: 5.42e-01

Confidence level: 6.55e-01

Nearest Neighbors from the Training Set

Image not found

4-Methylimidazolidine-2-thione

Measured: 10.0 Predicted: 4.59

Image not found

1,4-Dioxane

Measured: 5.01e-01 Predicted: 1.06

Image not found

Ethylene thiourea Measured: 1.82 Predicted: 1.85

Image not found

Paraldehyde Measured: 3.02 Predicted: 2.77

Image not found

N,N-Dimethylformamide Measured: 7.94e-01 Predicted: 1.12